FREE RADICAL CHEMISTRY OF COAL LIQUEFACTION. L. W. Vernon. Exxon Research and Engineering Company, P. O. Box 4255, Baytown, Texas, 77520.

In the direct hydrogenation of coal both donor hydrogen and molecular hydrogen play important roles. This report describes some studies which were made on a number of model structures thought to be present in coal, in order to obtain a better understanding of the function of these two hydrogen forms in the chemistry of coal liquefaction. When dibenzyl is pyrolyzed at 450°C, the products produced depend upon the hydrogen environment. In the absence of an external source of hydrogen the major products are toluene and stilbene. In the presence of a donor solvent such as tetralin the only major product is toluene. However, when the pyrolysis is carried out in the presence of molecular hydrogen, the major products are toluene, benzene and ethylbenzene. The product distribution is a function of hydrogen pressure. A simple reaction mechanism is proposed which is consistent with all these results. In this reaction scheme the initial reaction is the thermal cracking of the β bond to form benzyl radicals. The benzyl radical can be stabilized by abstraction of hydrogen from the donor solvent or from dibenzyl. With molecular hydrogen the stabilization reaction produces a hydrogen atom. The hydrogen atom can then promote the cracking of the α bond in dibenzyl to form benzene and ethylbenzene. Experiments with diphenyl give further evidence for the presence of hydrogen atoms in these systems.